

Drug targeting with OptFlux – *Piscirickettsia salmonis*

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search:		<input type="checkbox"/> Case sensitive	<input type="button" value="Options"/>
		<input type="checkbox"/> Whole word	
Reaction Id	Reaction Name	Lower Bound	Upper Bound
R_EX_cpd00007_e0	EX O2_e0	-2.0	1000.0
R_EX_cpd00161_e0	EX L-Threonine_e0	-5.0	1000.0
R_EX_cpd00108_e0	EX Galactose_e0	-5.0	1000.0
R_EX_cpd00023_e0	EX L-Glutamate_e0	-5.0	1000.0
R_EX_cpd00051_e0	EX L-Arginine_e0	-5.0	1000.0
R_EX_cpd00129_e0	EX L-Proline_e0	-5.0	1000.0
R_EX_cpd00067_e0	EX H_e0	-2.0	1000.0
R_EX_cpd00009_e0	EX Phosphate_e0	-2.0	1000.0

Fig1 – Condições ambientais ideais de *P.salmonis* com a função de objetivo de produção de biomassa.

Simulation Information

Method Name: FBA

Solution Type: OPTIMAL

Environmental Conditions: Env. Conditions

Objective Function

max: R_biomass0 = 0.70619452

Biomass value: 0.70619452

Net Conversions:

Consumption

Metabolite Id	Metabolite Name	Value
M_cpd00007_e0_c	O2_e0	1.94427
M_cpd00009_e0_c	Phosphate_e0	2.0
M_cpd00039_e0_c	L-Lysine_e0	0.20483
M_cpd00051_e0_c	L-Arginine_e0	1.1746
M_cpd00060_e0_c	L-Methionine_e0	0.06941
M_cpd00066_e0_c	L-Phenylalanine_e0	0.24706
M_cpd00067_e0_c	H_e0	1.55979
M_cpd00084_e0_c	L-Cysteine_e0	0.0351
M_cpd00107_e0_c	L-Leucine_e0	0.31478
M_cpd00108_e0_c	Galactose_e0	1.37765
M_cpd00119_e0_c	L-Histidine_e0	0.06623
M_cpd00156_e0_c	L-Valine_e0	0.18242
M_cpd00161_e0_c	L-Threonine_e0	0.96177
M_cpd00322_e0_c	L-Isoleucine_e0	0.23963

Production

Metabolite Id	Metabolite Name	Value
M_cpd00011_e0_c	CO2_e0	2.32073
M_cpd11416_c0_c	Biomass_c0	0.70619
M_cpd00073_e0_c	Urea_e0	0.02147
M_cpd00001_e0_c	H2O_e0	2.27475

Fig2 – Consumo e secreções de *P.salmonis* nas condições ambientais ideais.

A

Information	
Total Critical Reactions: 189	
Environmental Condition Name: Fontes de carbono • Energia	
Critical Reactions	
<input type="text"/> search :	<input type="checkbox"/> Case sensitive <input type="checkbox"/> Whole word
Options	
Critical Reactions Id	Critical Reactions Name
R_nn09_c0	biosynthesis purina
R_nn05332_c0	3R-3-Hydroxypalmitoyl-acyl-carrier-protein hydro-lyase c0
R_nn05183_c0	L-lysine
R_nn10213_c0	stearoyl-1-acylglycerol-3-phosphate O-acyltransferase c0
R_nn05343_c0	Octanoyl-acyl-carrier protein malonyl-acyl-carrier-protein c0
R_nn08311_c0	CDP-diacylglycerol synthetase n-C18 0 c0
R_nn10_c0	biosynthesis pirimidina
R_nn00800_c0	N6-1 2-DicarbonylAMP AMP-lyase c0
R_nn03917_c0	sedoheptulose 7-phosphate isomerase c0
R_nn21_c0	agua
R_nn00102_c0	Carbonic acid hydro-lyase c0
R_nn05184_c0	L-methionine
R_nn09225_c0	rhmannosyltransferase I LPS core biosynthesis c0
R_nn00342_c0	L-Asparagine amidohydrolase c0
R_nn09202_c0	Phosphatidylserine decarboxylase n-C18 0 c0
R_nn03918_c0	D-glycero-D-manno-heptose 7-phosphate kinase c0
R_nn05229_c0	NCAIR synthetase and NCAIR mutase c0
R_nn01117_c0	D-Arabinose-5-phosphate ketol-isomerase c0
R_nn01520_c0	5 10-Methylenetetrahydrofolate dUMP C-methyltransferase c0
R_nn01644_c0	L-Aspartate 4-semialdehyde hydro-lyase adding pyruvate and c0
R_nn00834_c0	IMP NAD oxidoreductase c0
R_nn01485_c0	D-Glucosamine 1-phosphate 1 6-phosphomutase c0
R_nn05331_c0	3R-3-Hydroxybutanoyl-acyl-carrier-protein hydro-lyase c0
R_nn08712_c0	heptosyltransferase III LPS core synthesis c0
R_nn05459_c0	stearyl-ACP acyl-carrier-protein transferase c0
R_nn08711_c0	heptosyltransferase II LPS core synthesis c0
R_nn20_c0	amylase a g
R_nn03916_c0	D-glycero-D-manno-hepese 1-phosphate adenylyltransferase c0
R_nn19_c0	Phosphatidylserine decarboxylase n-C18 a g
R_nn05322_c0	Bu-yl-acyl-carrier protein malonyl-CoA c0
R_nn02213_c0	3-Dehydroquinate hydro-lyase c0
R_nn03164_c0	UDP-N-acetylmuramoyl-L-alanyl-D-glutaryl-meso-2 6- c0
R_nn05333_c0	3R-3-Hydroxybutanoyl-acyl-carrier-protein hydro-lyase c0
R_nn01643_c0	L-Aspartate 4-semialdehyde NADP oxidoreductase phosphorylating c0
R_nn05344_c0	Tetradecanoyl-acyl-carrier protein malonyl-acyl-carrier-protein c0
R_nn02212_c0	2-Dehydro-3-deoxy-D-arabino-heptonate 7-phosphate phosphate-lyase c0
R_nn00917_c0	Xanthosine-5-phosphate L-glutamine amido-ligase AMP-forming c0
R_nn03130_c0	UDP-2 3-bis(3-hydroxytetradecanoyl)glucosamine diphosphatase c0
R_nn08954_c0	3-deoxy-D-manno-oculosonic acid transferase III LPS core biosynthesis c0
R_nn05185_c0	L-phenylalanine

B

Critical Genes	
<input type="text"/> search :	<input type="checkbox"/> Case sensitive <input type="checkbox"/> Whole word
Options	
Critical Genes	
00000000.0.peg.1190	
00000000.0.peg.461	
00000000.0.peg.463	
00000000.0.peg.742	
00000000.0.peg.745	
00000000.0.peg.746	
00000000.0.peg.505	
00000000.0.peg.1001	
00000000.0.peg.351	
00000000.0.peg.354	
00000000.0.peg.631	
00000000.0.peg.358	
00000000.0.peg.512	
00000000.0.peg.359	
00000000.0.peg.514	
00000000.0.peg.519	
00000000.0.peg.1806	
00000000.0.peg.1496	
00000000.0.peg.1013	
00000000.0.peg.888	
00000000.0.peg.1268	
00000000.0.peg.650	
00000000.0.peg.773	
00000000.0.peg.816	
00000000.0.peg.817	
00000000.0.peg.1035	
00000000.0.peg.1837	
00000000.0.peg.1337	
00000000.0.peg.1058	
00000000.0.peg.328	
00000000.0.peg.725	
00000000.0.peg.848	
00000000.0.peg.849	
00000000.0.peg.1348	
00000000.0.peg.691	
00000000.0.peg.295	
00000000.0.peg.570	
00000000.0.peg.457	
00000000.0.peg.578	
00000000.0.peg.458	

Fig3 – Reações críticas (A) e Genes críticos (B) de *P.salmonis*.